

# Seminar on Condensed Matter Theory

Group of Theoretical Physics at the Department of Condensed Matter Physics  
of Charles University has a pleasure to invite you to attend the seminar

**on 9 May 2019 at 13:00**

at Faculty of Mathematics and Physics of Charles University, Ke Karlovu 5, 121 16 Praha 2

**Seminar room F052**



## Ing. Matúš Dubecký, Ph.D.

*Department of Physics, University of Ostrava, Ostrava, Czech Republic; ATRI, Slovak  
University of Technology, Trnava, Slovakia*

## Fractional charge by fixed-node diffusion Monte Carlo

Fixed-node diffusion Monte Carlo (FNDMC) is a stochastic quantum many-body method that has a great potential in electronic structure theory. We examine how FNDMC satisfies exact constraints, linearity and derivative discontinuity of total energy  $E(N)$  vs. fractional electron number  $N$ , if combined with mean-field trial wave functions that miss such features. H and Cl atoms with fractional charge reveal that FNDMC is well able to restore the piecewise linearity of  $E(N)$ . The method uses ensemble and projector ingredients to achieve the correct charge localization. Water-solvated Cl-complex illustrates superior performance of FNDMC for charged noncovalent systems.

See preprint at arXiv:1903.12378 [physics.chem-ph].

